

Claims

1. A method for simulation of at least one biological and/or chemical reaction pathway comprising:
 - preparing a map of at least one biological and/or chemical reaction pathway;
 - constructing at least one set of binding and reaction equation from the pathway map;
 - constructing at least one set of concentration equation for molecules of the pathway map;
 - constructing an electronic circuit corresponding to every set of equation; and
 - determining simulation of pathway by measuring voltage at two or more connection points of the circuit.
2. The method of claim 1, wherein the binding, reaction and/or concentration equation is a linear or non-linear first- or second-order ordinary differential equation (ODE).
3. The method of claim 1, wherein the binding, reaction and/or concentration equation is a non-linear first-order ordinary differential equation (ODE).
4. The method of claim 1, wherein the electronic circuit comprises at least one of the following circuit units: linear protein/molecule concentration $\pm kx_i$ unit; protein/molecule concentration power $\pm kx_i^a$ unit; ligand-protein concentration product $\pm Lx_i$ unit; ligand-protein concentration power product $\pm kLx_i^a$ unit; protein-protein concentration product $\pm kx_i x_j$ unit; protein-protein concentration power product $\pm kx_i^a x_j^b$ unit; stochastic rate constant generator unit that replaces a forward/reverse binding/reaction rate constant k by a stochastic value; and

wherein, k is a forward/reverse binding/reaction rate constant, L the concentration of a ligand, x_i and x_j are the concentration of protein/molecule x_i and x_j respectively, a and b are order of power of x_i and x_j .

5

5. The method of claim 1, further comprising maintaining the voltage level of the circuit between two fixed voltage values.

10

6. The method of claim 5, wherein the voltage level of the circuit is maintained between two fixed voltage values by:

multiplying scaling factors to the concentration equation;

applying at least one resistor and/or amplifier at one or more connection point of the circuit, thereby scaling-down or scaling-up the voltage of one or more segment of the circuit; and/or

15

applying automatic gain control circuits.

7. The method of claim 1, further comprising adding at least one unit circuit comprising an electronic random noise generator and/or a multiplier amplifier at one or more connection point of the circuit.

20

8. The method of claim 1, further comprising determining the effect of at least one drug comprising adding at least one circuit unit associated with a receptor protein at one or more connection point of the circuit.

25

9. The method of claim 1, further comprising determining deficiency, mutation and/or deletion of at least one protein of the biological pathway, comprising setting a voltage ceiling, a voltage range and/or a fixed voltage at one or more connection point of the circuit.

10. The method of claim 1, wherein the biological pathway comprises at least one object, and wherein the object is protein, nucleic acid, ligand, substrate, inhibitor or antagonist, activator or agonist, reactant and/or reaction product.
- 5 11. An electronic circuit system for the simulation of at least one biological and/or chemical reaction pathway, comprising at least one electronic circuit representing a set of binding, reaction and/or concentration equation.
- 10 12. The electronic circuit system of claim 11, wherein the binding, reaction and/or concentration equation is a linear or non-linear first- or second-order ordinary differential equation (ODE).
- 15 13. The electronic circuit system of claim 11, wherein the electronic circuit comprises at least one the following circuit units: linear protein/molecule concentration $\pm kx_i$ unit; protein/molecule concentration power $\pm kx_i^a$ unit; ligand-protein concentration product $\pm Lx_i$ unit; ligand-protein concentration power product $\pm kLx_i^a$ unit; protein-protein concentration product $\pm kx_i x_j$ unit; protein-protein concentration power product $\pm kx_i^a x_j^b$ unit; stochastic rate constant generator unit that replaces a forward/reverse binding/reaction rate constant k by a stochastic value; and
- 20 wherein, k is a forward/reverse binding/reaction rate constant, L the concentration of a ligand, x_i and x_j are the concentration of protein/molecule x_i and x_j respectively, a and b are order of power of x_i and x_j respectively.
- 25 14. A method for molecular dynamics simulation of biomolecules and/or nano-molecular systems comprising:

constructing at least one set of equation representing the molecular dynamics of at least one molecule of the biomolecules and/or the nano-molecular systems;

constructing an electronic circuit representing every set of equation; and

5 determining molecular dynamics simulation by measuring voltage at two or more connection points of the circuit.

15. The method of claim 14, wherein the equation is a linear or non-linear second order ordinary differential equation (ODE).

10 16. The method of claim 14, wherein the electronic circuit comprises at least one atom-position circuit unit, wherein the atom-position circuit unit represents the position of an atom of a molecule or a molecular system.

17. The method of claim 16, wherein the atom-position circuit unit comprises at least one atom-atom interaction circuit subunit, the atom-atom
15 interaction circuit subunit representing a sub-unit of atom-atom interactions within a molecule or a molecular system and comprising at least one of: internal bond stretch, angle bending, torsion, non-bonded unit; bond stretch, angle bending, and torsion unit; between at least two nearest sub-unit of a molecule.

20 18. The method of claim 17, wherein each atom-atom interaction circuit subunit represents a term in the molecular dynamics equation, and wherein the atom-atom interaction circuit subunit comprises at least one of the following: bond stretch x unit, bond stretch y unit, bond stretch z unit, angle bending x type-A unit, angle bending x type-B unit, angle bending y
25 type-A unit, angle bending y type-B unit, angle bending z type-A unit, angle bending z type-B unit, torsion x type-A unit, torsion x type-B unit, torsion y type-A unit, torsion y type-B unit, torsion z type-A unit, torsion z type-B

unit, non-bonded x unit, non-bonded y unit, non-bonded z unit, hydrogen-bond x unit, hydrogen-bond y unit, and hydrogen-bond z unit; and

wherein x, y, and z represent the coordinates of each atom of the molecule, and type-A represents the case of the atom being in the middle-position of an angle bending or torsion connection with other atoms, and
 5 type-B represents the case of the atom being in the end-position of an angle bending or torsion connection with other atoms.

19. The method of claim 14, further comprising maintaining the voltage level in the circuit between two fixed voltage values.

10 20. The method of claim 19, wherein x, y and z represent the coordinate of the molecule, and the voltage level of the circuit is maintained between two fixed voltage values by:

applying scaling factors to the x, y and z coordinates and to the molecular dynamic equation;

15 applying at least one resistor and/or amplifier at one or more connection point of the circuit, thereby scaling-down or -up the voltage of one or more segment of the circuit; and/or

applying automatic gain control circuits.

20 21. The method of claim 14, wherein the biomolecule comprises amino acids, nucleotides and/or organic molecules.

22. A circuit group representing the interaction pattern in the chemical structure of a molecule or a sub-unit of interaction pattern in the chemical structure of a molecule comprising:

25 a bond stretch connection between each atom pair of the molecule covalently bonded to each other;

an angle bending connection pair between a first atom and other two atoms;

a torsion connection bundle between a first atom and other three atoms;
and

- 5 a non-bonded connection between each atom pair whose atoms are at least four bonds away from each other.

23. A circuit unit comprising at least one circuit group of claim 22.

- 10 24. An electronic circuit comprising at least one circuit unit, the circuit unit comprising at least one circuit group, the circuit group representing a sub-unit of interaction pattern in the chemical structure of a molecule and comprising internal bond stretch, angle bending, torsion, non-bonded units; and/or bond stretch, angle bending, and/or and torsion units;
15 between at least two nearest sub-unit of a molecule.

25. The electronic circuit of claim 24, wherein each circuit unit represents a term in the molecular dynamic equation, and wherein the circuit unit comprises at least one of the following: bond stretch x unit, bond stretch y unit, bond stretch z unit, angle bending x type-A unit, angle bending x type-B unit, angle bending y type-A unit, angle bending y type-B unit, angle bending z type-A unit, angle bending z type-B unit, torsion x type-A unit, torsion x type-B unit, torsion y type-A unit, torsion y type-B unit, torsion z type-A unit, torsion z type-B unit, non-bonded x unit, non-bonded y unit,
20 non-bonded z unit, hydrogen-bond x unit, hydrogen-bond y unit, and hydrogen-bond z unit; and wherein x, y, and z represent the coordinates of each atom of the molecule, and type-A unit represents the case of the atom being in the middle-position of an angle bending or torsion connection with other atoms, and type-B represents the case of the atom
25

being in the end-position of an angle bending or torsion connection with other atoms.

26. A method for the manufacture of an electronic circuit representing at least one biomolecule and/or nano-molecular system, the electronic circuit comprising at least a unit circuit comprising at least a circuit group, wherein the circuit group represents a sub-unit of interaction pattern in the chemical structure of a molecule or a molecular system comprising:
- introducing a bond stretch between each atom of a pair of atoms covalently bonded to each other;
 - introducing an angle bending connecting pair between a first atom and other two atoms;
 - introducing a torsion connection bundle between a first atom and other three atoms; and
 - introducing a non-bonded connection between each atom pair whose atoms are at least four bonds away from each other.